5-3-2014

A First-Principle Study of Small Neutral and Anionic Silver Halide Clusters

Erik Langholz
Valparaiso University, erik.langholz@valpo.edu

Stephen Place
Valparaiso University

John Eric Tiessen
Valparaiso University

Haiying He
Valparaiso University

Stan Zygmunt
Valparaiso University

A First-Principle Study of Small Neutral and Anionic Silver Halide Clusters

Erik Langholz, Stephen Place, John Eric Tiessen, Haiying He, Stan Zygmunt

Departmental Affiliation: Physics and Astronomy
College of Arts and Sciences

Silver halide is a material that was traditionally used in photographic films. In recent years, there has been a revived interest in using small clusters of silver halides for photocatalytic and photovoltaic applications. We present the results of a theoretical study of neutral and anionic AgnXn (X = F, Cl, and Br, and n = 1-6) clusters. Quantum-mechanical calculations were performed using Density Functional Theory (DFT) in search of the lowest-energy isomers of the neutral and anionic clusters with applied symmetry constraints. The optimal configurations are compared across the series of AgF, AgCl, and AgBr. The variation in binding energies, bond lengths, charge distributions, HOMO-LUMO gaps, and electron affinities will be discussed as a function of cluster size and composition. The study of these clusters allows us to gain a better understanding of the structure and function of these materials in current and future applications.

Information about the Authors:
John Eric Tiessen is currently a physics major at Valparaiso University. He plans on going to graduate school after completing his undergraduate degree and would like to go into computational work. Stephen Place is a sophomore physics major from Goshen, Indiana. Stephen intends to pursue graduate school after graduation. Erik Langholz is a sophomore mechanical engineering major from Kaiserslautern, Germany. Upon graduating, Erik plans to either become a pilot in the U.S. Air Force or go to graduate school for engineering or applied physics.

Faculty Sponsor: Dr. Haiying He, Dr. Stan Zygmunt

Student Contact: erik.langholz@valpo.edu